

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

HCH consists of eight isomers (Safe 1993). Only γ -HCH, α -HCH, β -HCH, and δ -HCH are of commercial significance and considered in this profile. The pesticide lindane refers to products that contain >99% γ -HCH. The α -, β -, and δ -isomers, as well as technical-grade HCH are not synonymous with lindane (Farm Chemicals Handbook 1993). Technical-grade HCH is not an isomer of HCH, but rather a mixture of several isomers; it consists of approximately 60–70% α -HCH, 5–12% β -HCH, 10–15% γ -HCH, 6–10% δ -HCH, and 3–4% ϵ -HCH (Kutz et al. 1991). Information regarding the chemical identities of γ -HCH, α -HCH, β -HCH, and δ -HCH is located in Table 4-1.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of γ -HCH, α -HCH, β -HCH, and δ -HCH is located in Table 4-2.

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Table 4-1. Chemical Identity of Hexachlorocyclohexane Isomers^a

Characteristic	γ -hexachlorocyclohexane	α -hexachlorocyclohexane
Synonym(s)	Lindane; 1-alpha, 2-alpha, 3-beta, 4-alpha, 5-alpha, 6-beta-hexachlorocyclohexane; benzene hexachloride-gamma-isomer; BHC; cyclohexane 1,2,3,4,5,6-hexachloro-gamma-isomer; ENT 7796; gamma-benzene hexachloride; gamma-BHC; gamma-hexachlorocyclohexane; gamma-1,2,3,4,5,6-hexachlorocyclohexane; gamma-HCH; gamma-lindane; HCH; HCCH; hexachlorocyclohexane, gamma-isomer; 1,2,3,4,5,6-hexachlorocyclohexane, gamma-isomer ^{a,b}	1-alpha, 2-alpha, 3-beta, 4-alpha, 5-beta, 6-beta-benzene-trans-hexachloride; alpha-1,2,3,4,5,6-hexachlorocyclohexane; alpha-benzene hexachloride; alpha-BHC; alpha-HCH; alpha-hexachloran; alpha-hexachlorane; alpha-hexachlorocyclohexane; alpha-lindane; benzenehexachloride-alpha-isomer; cyclohexane 1,2,3,4,5,6-(alpha, DL); cyclohexane 1,2,3,4,5,6-hexachloro, alpha-; cyclohexane 1,2,3,4,5,6-hexachloro-, alpha-isomer; cyclohexane, alpha-1,2,3,4,5,6-hexachloro; ENT 9232 ^{a,b}
Registered trade name(s)	Etan 3G (Diachem S.P.A.); Forlin; Gamaphex; Isotox (Chevron Chemical Co.); Germate Plus (Gustafson Inc.); Gamma-Mean 400 and Gamma Mean L. (Oregon-California Chemicals, Inc.); Hammer (Exsin Industries); Lindagam; Novigam; Silvanol ^c ; Kwell (pharmaceutical shampoo/lotion) ^d .	No data
Chemical formula	$C_6H_6Cl_6$ ^a	$C_6H_6Cl_6$ ^b
Chemical structure		
Identification numbers:		
CAS registry	58-89-9	319-84-6
NIOSH RTECS	GV4900000	GV3500000
EPA hazardous waste	U129; D013	No data
OHM/TADS	7216531	810002
DOT/UN/NA/IMCO shipping	NA 2761 lindane; IMCO 6.1 lindane; UN 2761, organochlorine pesticides, solid toxic, not otherwise specified	No data
HSDB	646	6029
NCI	C00204	No data

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Table 4-1. Chemical Identity of Hexachlorocyclohexane Isomers^a

Characteristic	β -hexachlorocyclohexane	δ -hexachlorocyclohexane
Synonym(s)	1-alpha, 2-beta, 3-alpha, 4-beta, 5-alpha, 6-beta-hexachlorocyclohexane; beta 1,2,3,4,5,6-hexachlorocyclohexane; beta-benzenehexachloride; beta-BHC; beta HCH; beta-hexachloran; beta-hexachlorobenzene; beta-lindane; cyclohexane, 1,2,3,4,5,6-hexachloro-, beta-; cyclohexane, 1,2,3,4,5,6-hexachloro-, beta-isomer; cyclohexane, 1,2,3,4,5,6-hexachloro-, trans-; cyclohexane, beta-1,2,3,4,5,6-hexachloro-; ENT 9233; trans-alpha-benzenehexachloride ^{a,b}	1-alpha,2-alpha,3-alpha, 4-beta, 5-alpha, 6-beta-hexachlorocyclohexane; cyclohexane, 1,2,3,4,5,6-hexachloro-, delta-isomer; cyclohexane, delta-1,2,3,4,5,6-hexachloro-; delta-(AEEEE)-1,2,3,4,5,6-hexachlorocyclohexane; delta-benzenehexachloride; delta-BHC; delta-HCH; delta-1,2,3,4,5,6-hexachlorocyclohexane; delta-lindane; ENT 9234 ^{a,b}
Registered trade name(s)	No data	No data
Chemical formula	$C_6H_6Cl_6$ ^a	$C_6H_6Cl_6$ ^a
Chemical structure		
Identification numbers:		
CAS registry	319-85-7	319-86-8
NIOSH RTECS	GV4375000	GV4550000
EPA hazardous waste	No data	No data
OHM/TADS	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data
HSDB	6183	6184
NCI	No data	No data

^aAll information obtained from HSDB 1997 except where noted.^bRTECS 1993^cFarm Chemicals Handbook 1993^dBudavari et al. 1989

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

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Table 4-2. Physical and Chemical Properties of Hexachlorocyclohexane Isomers

Property	γ -hexachlorocyclohexane	α -hexachlorocyclohexane	β -hexachlorocyclohexane	δ -hexachlorocyclohexane
Molecular weight	290.83 ^a	290.83 ^a	290.83 ^a	290.83 ^a
Color	White ^b	Brownish to white ^c	No data	No data
Physical state	Crystalline solid ^d ; monoclinic prisms ^b	Crystalline solid ^c ; monoclinic prisms ^a	Crystalline solid ^{a,d}	Fine plates ^{a,b}
Melting point	112.5 °C ^{a,e}	159–160 °C ^a	314–315 °C ^a	141–142 °C ^a
Boiling point	323.4 °C at 760 mmHg ^c	288 °C at 760 mmHg ^c	60 °C at 0.5 mmHg ^a	60 °C at 0.36 mmHg ^a
Density (g/cm ³)	1.89 at 19 °C ^f	1.87 at 20 °C ^a	1.89 at 19 °C ^a	No data
Odor	Slightly musty odor ^c	Phosgene-like odor ^c	No data	No data
Odor threshold:				
Water	12 mg/kg ^g	0.88 ppm for unspecified purity ^h	0.00032 mg/kg ^g	No data
Air	No data	No data	No data	No data
Solubility:				
Water	17 ppm ⁱ ; insoluble in water ^c	10 ppm ^j ; 69.5 mg/L at 28 °C ^k	5 ppm ^j	10 ppm ^j
Organic solvents	6.4 g/100 g in ethanol; 20.8 g/100 g in ether; 28.9 g/100 g in benzene ^j	Soluble in alcohol ^k ; 1.8 g/100 g in ethanol ^j ; 6.2 g/100 g in ether ^j	1.1 g/100 g in ethanol; 24.4 g/100 g in ethanol; 1.8 g/100 g in ether; 1.9 g/100 g in benzene ^j	35.4 g/100 g in ether; 41.4 g/100 g in benzene ^j
Partition coefficients:				
Log K _{ow}	3.72 ^l	3.8 ^l	3.78 ^l	4.14 ^l
Log K _{oc}	3.0 ^m ; 3.57 ^f	3.57 ^f	3.57 ^m	3.8 ^f
Vapor pressure	4.2x10 ⁻⁵ mmHg at 20 °C ^c	4.5x10 ⁻⁵ mmHg at 25 °C ^c	3.6x10 ⁻⁷ at 20 °C ^c	3.5x10 ⁻⁵ at 25 °C ^c
Henry's law constant	3.5x10 ⁻⁶ ^c	6.86x10 ⁻⁶ ^c	4.5x10 ⁻⁷ ^{m,n}	2.1x10 ⁻⁷ ^{o,p}
Autoignition temperature	Not flammable ^c	No data	No data	No data
Flashpoint	Approximately 150 °F (closed cup) ^c	No data	No data	No data
Flammability limits	Not flammable ^c	No data	No data	No data
Conversion factors ^q	ppm to mg/m ³ in air (20°C): ppm x 4.96 = mg/m ³ ; mg/m ³ to ppm in air (20°C): mg/m ³ x 0.20 = ppm			
Explosive limits	No data	No data	No data	No data

^aLide 1991^eBudavari et al. 1989ⁱHollifield 1979^lHansch and Leo 1995^oPankow et al. 1984^bKirk-Othmer 1985^fWeiss 1986^jClayton and Clayton^mRipping 1972^pEPA 1982^cHSDB 2003^gVerschueren 1983ⁿVeith et al. 1979^qSame for all isomers^dIARC 1979^hFazzalari 1978^kKuihara et al. 1973